Hosung Seo, Ph.D.

Postdoctoral Fellow at the Argonne National Lab and the University of Chicago

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EDUCATION

Ph.D. in Physics, The University of Texas at Austin, Austin, TX, USA 2013

Field: Condensed Matter Theory

Concentration: Computational Materials Theory

Adviser: Alexander A. Demkov

Dissertation Title: Functional Oxide Heterostructures on Semiconductors

M.S. in Physics, Northwestern University, Evanston, IL, USA 2008

B.S. in Physics, Seoul National University, Seoul, Korea 2006

FELLOWSHIPS

William Powers, Jr. Presidential Fellowship, The University of Texas at Austin, Austin, TX, USA 09/2012

- One of the highest honors awarded to a graduate researcher at the University
- Provided dissertation support throughout the academic year

Biedenharn Graduate Fellowship, University of Texas at Austin, TX, Austin, USA 08/2008

- Recruiting fellowship awarded by the physics department to attract an outstanding graduate researcher

University and Huang Fellowship, Northwestern University**,** Evanston, IL, USA 09/2006

- Recruiting fellowship awarded by the university to attract an outstanding graduate researcher

ACADEMIC AWARDS AND HONORS

APS DCOMP Travel Award, American Physical Society (APS) 03/2017

- Provided a travel support for an invited talk about spin qubits in semiconductors

Young Scientist Award, The 39th Conference on the Physics and Chemistry of Surfaces and Interfaces, Santa Fe, NM, USA 01/2012

- In recognition of excellence in research on correlated magnetic oxide $LaCoO_3$

RESEARCH EXPERIENCE

Postdoctoral Researcher, The Group of Giulia Galli, Ph.D.

Argonne National Laboratory (MSD) & University of Chicago (IME), Chicago, IL, USA 12/2016 -

University of Chicago, Institute for Molecular Engineering, Chicago, IL, USA 2014 - 2016

University of California, Department of Chemistry, Davis, CA, USA 2013 - 2014

- Collaborated with the group of David Awschalom to explore the quantum decoherence of divacancy spins in silicon carbide. Suggested that developing spin qubits in complex poly-atomic crystals would be a promising route to realize novel, multifunctional, quantum systems.
- Proposed a number of new 'portable' strategies to implement defect spin qubits in piezoelectric semiconductors in the pursuit of scalable hybrid quantum systems.
- Exploring new quantum platforms in complex oxides for novel quantum information processing in collaborations with researchers at the Argonne National Lab.
- Collaborating with the group of Yuan Ping to identify the origin behind the superior photocatalytic property of defect-engineered $BiVO_4$.
- Investigating new controlled ways of optical gating for 2-dimensional materials systems on complex oxides.

Graduate Researcher, The Group of Alexander Demkov, Ph.D. 09/2008 - 08/2013

The University of Texas at Austin**,** Physics Department, Austin, TX, USA

- Investigated emergent properties in correlated oxide heterostructures. Explained most of the key experimental features of strained $LaCoO_3$ on $SrTiO_3$(001) that have remained unresolved. Showed that tensile-strained $LaCoO_3$ develop a novel high spin – low spin mixed state.
- Studied epitaxial oxide heterostructures as energy materials. Analyzed the photocatalytic anatase $TiO_2/SrTiO_3$ and the visible-light photo-active $CoO/SrTiO_3$ (001) hetero-interfaces. Explored the Schottky barrier formation in the system of Pt nano-clusters on $SrTiO_3$(001).
- Studied monolithic integration of functional oxides on semiconductors. Explained the unusual features found in the Si 2*p* surface core-level spectrum of the Sr/Si(001) Zintl template.
- Identified the origin of a number of highly debated ARPES features of Ge(001) and Si(001). Showed that the surface state that determines the charge neutrality level, and thus the Schottky barrier height in Si, is a surface resonance in Ge.

Graduate Researcher, Laboratory of Manijeh Razeghi, Ph.D. 12/2006 - 12/2007

Northwestern University**,** Physics Department, Evanston, IL, USA

- Investigated epitaxial self-assembled InAs quantum dots embedded in III-V semiconductor quantum-well structures for applications in room-temperature infrared optical sensing and imaging. Performed materials growths, characterizations, device fabrications, and analysis.

RESEARCH INTERESTS

Main areas: Condensed matter theory, computational materials physics, applied physics

Research directions of interest include (but are not limited to):

- Theory-experiment collaborative research
- Solid-state quantum information: devices, applications, and theory of decoherence
- Quantum spintronics: spin-lattice hybrid systems and quantum sensing
- Beyond Moore's law: advanced electronics based on multi-functional heterostructures
- Materials physics for next-generation energy materials
- Theoretical spectroscopy: ARPES, XPS, STEM/EELS, EPR/NMR, and STM/STS

TECHNICAL AND SPECIALIZED SKILLS

Computer programming: C/C++, scientific Python, Matlab, shell scripting

- Implemented a cluster-correlation expansion (CCE) method to solve for the decoherence dynamics of a spin qubit coupled to a strongly correlated quantum bath of nuclear spins in a semiconductor.

***Ab initio* calculation codes:** VASP, Quantum Espresso, WEST (GW many body perturbation theory)

GRANT ACTIVITIES

1. Marco Govoni, Alex P. Gaiduk, and **Hosung Seo**, *Computational engineering of defects in soft and hard materials for energy and quantum information applications,* 2016 ASCR Leadership Computing Challenge (ALCC) Award (2016).
   - Received 53.7 million hours on MIRA at Argonne National Laboratory
   - Highlighted by the Argonne Leadership Computing Facility [Link to the article)

PUBLICATIONS (*in preparation*)

1. **Hosung Seo**, He Ma, Marco Govoni, and Giulia Galli, *Portable defect qubit platforms in wide-gap semiconductors with large spin-strain coupling* (2017).
2. **Hosung Seo***, Yuan Ping*, Nicholas Brawand, Matthew Goldey, and Giulia Galli, *Microscopic origin of the superior photocatalytic activity of defect-engineered $BiVO_4$* (2017).
   - (*) Co-first authors
3. **Hosung Seo** and Giulia Galli, *First-principles theory of nitrogen vacancy in aluminum nitrides* (2017).
4. He Ma, **Hosung Seo**, and Giulia Galli, *First-principles simulations of transition metal ions in silicon as potential quantum bits* (2017).

PUBLICATIONS

1. **Hosung Seo**, Abram L. Falk, Paul V. Klimov, Kevin C. Miao, Giulia Galli, and David Awschalom, *Quantum decoherence dynamics of divacancy spins in silicon carbide*, Nature Communications **7**, 12935 (2016).
   - Highlighted in the University of Chicago News*: Exceptionally robust quantum states found in industrially important semiconductor*
   - Highlighted by the Research Computing Center of the University of Chicago: *The Sweet Spot*
   - Highlighted by the US Department of Energy: *Supercomputers for Quantum Computers*
2. Kurt D. Fredrickson, **Hosung Seo**, and Alexander A. Demkov, *Mechanism of oxidation protection of the Si(001) surface by sub-monolayer Sr template,* Journal of Applied Physics **120**, 065301 (2016).
3. **Hosung Seo**, Marco Govoni, and Giulia Galli, *Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies*, Nature Scientific Reports **6**, 20803 (2016).
   - Highlighted by the Research Computing Center of the University of Chicago: *From the Bottom Up*

- Highlighted by the Lawrence Berkeley National Laboratory: *Could Aluminum Nitride Produce Quantum Bits?* Also appeared at the University of Chicago news, the University of Chicago IME news, Sciencedaily, Science Bulletin, and Phys.org.
- Highlighted by the US Department of Energy: *Supercomputers for Quantum Computers*
- Highlighted by the Argonne Leadership Computing Facility [Link to the article].

4. **Hosung Seo** and Alexander A. Demkov, *Early stages of the Schottky barrier formation in sub-monolayer Pt on $SrTiO_3$ (001),* Physical Review B **92**, 245301 (2015).
5. William F. Koehl, ***Hosung Seo**, Giulia Galli, and David A. Awschalom, *Designing defect spins for wafer-scale quantum technologies*, MRS Bulletin **40**, 1146-1153 (2015).
   - Primary theoretical author (*)
   - A special 40th anniversary issue on Materials & Engineering: Propelling Innovation
   - Highlighted in the feature article of University of Chicago Institute for Molecular Engineering
6. **Hosung Seo** and Alexander A. Demkov, *Band alignment in visible-light photo-active CoO/$SrTiO_3$ (001) heterostructures,* Journal of Applied Physics **116**, 245305 (2014).
7. **Hosung Seo**, Richard C. Hatch, Patrick Ponath, Miri Choi, Agham B. Posadas, and Alexander A. Demkov, *Critical differences in the surface electronic structure of Ge(001) and Si(001): Ab initio theory and angle-resolved photoemission spectroscopy,* Physical Review B **89**, 115318 (2014).
8. Richard C. Hatch, Kurt D. Fredrickson, Miri Choi, Chungwei Lin, **Hosung Seo**, Agham B. Posadas, and Alexander A. Demkov, *Surface electronic structure for various surface preparations of Nb-doped $SrTiO_3$ (001),* Journal of Applied Physics **114**, 103710 (2013).
9. Thong Q. Ngo, Agham B. Posadas, ***Hosung Seo**, Son T. Hoang, Martin D. McDaniel, Dirk Utess, Dina Triyoso, Alexander A. Demkov, and John G. Ekerdt, *Atomic Layer Deposition of Epitaxial Photoactive CoO, CoO/$SrTiO_3$, and CoO/TiO_2 on Si (001) for Water Splitting in Visible Light,* Journal of Applied Physics **114**, 084901 (2013).
   - Primary theoretical author (*)
10. **Hosung Seo**, Miri Choi, Agham B. Posadas, Richard C. Hatch, and Alexander A. Demkov, *Combined in-situ photoemission experiment and density functional theory for the Sr Zintl template for oxide heteroepitaxy on Si(001),* Journal of Vacuum Science & Technology B **31**, 04D107 (2013).
11. Alexander A. Demkov, Agham B. Posadas, **Hosung Seo**, Miri Choi, Kristy J. Kormondy, Patrick Ponath, Richard C. Hatch, Martin. D. McDaniel, Thong Ngo and John G. Ekerdt, *(Invited) Monolithic integration of oxides on semiconductors,* ECS Transactions, **54** (1), 255 (2013).
12. Miri Choi, Agham B. Posadas, ***Hosung Seo**, Richard C. Hatch, and Alexander A. Demkov, *Charge transfer in Sr Zintl templates for epitaxial oxide growth on Si(001),* Applied Physics Letters **102**, 031604 (2013).
   - Primary theoretical author (*)
13. **Hosung Seo**, Agham B. Posadas, Chandrima Mitra, Alexander V. Kvit, Jamal Ramdani, and Alexander A. Demkov, *Band alignment and electronic structure of the anatase TiO_2/$SrTiO_3$ (100) heterostructure integrated on Si(100),* Physical Review B **86**, 075301 (2012).
14. **Hosung Seo**, Agham B. Posadas and Alexander A. Demkov, *Strain-induced spin state transition and superexchange in $LaCoO_3$,* Physical Review B **86**, 014430 (2012).
15. **Hosung Seo**, Agham B. Posadas and Alexander A. Demkov, *First-principles study of the growth thermodynamics of Pt on $SrTiO_3$ (001),* Journal of Vacuum Science & Technology B **30**, 04E108 (2012).

16. Alexander A. Demkov, **Hosung Seo**, Xiaodong Zhang, and Jamal Ramdani, *Using Zintl-Klemm intermetallics in oxide-semiconductor heteroepitaxy,* Applied Physics Letters **100**, 071602 (2012).
17. **Hosung Seo** and Alexander A. Demkov, *First-principles study of polar $LaAlO_3$ (001) surface stabilization by point defects,* Physical Review B **84**, 045440 (2011).
18. Alexander A. Demkov, Agham B. Posadas, **Hosung Seo** and Jeakwang Lee, *(Invited) Properties of oxides heterostructures,* ECS Transactions, **41**, 275 (2011).
19. Alexander A. Demkov, Agham B. Posadas, **Hosung Seo**, Jaekwang Lee, and Na Sai, *Emerging physics of oxide heterostructures,* Physica Status Solidi (b) **248**, 2076 (2011).
20. A. Posadas, M. Berg, *__Hosung Seo__, D. J. Smith, A. P. Kirk, D. Zhernokletov, R. M. Wallace, A. de Lozanne, A. A. Demkov, *Strain-induced ferromagnetism in $LaCoO_3$: Theory and growth on Si (100),* Microelectronic Engineering **88**, 1444 (2011).
    - Primary theoretical author (*)
21. A. Posadas, M. Berg, *__Hosung Seo__, A. de Lozanne, A. A. Demkov, D. J. Smith, A. P. Kirk, D. Zhernokletov, and R. M. Wallace, *Epitaxial integration of ferromagnetic correlated oxide $LaCoO_3$ with Si(100),* Applied Physics Letters **98**, 053104 (2011).
    - Primary theoretical author (*)
22. Stanley Tsao, Hochul Lim, **Hosung Seo**, Wei Zhang and Manijeh Razeghi, *InP-based quantum-dot infrared photodetectors with high quantum efficiency and high temperature imaging*, IEEE Sensors Journal **8**, 936 (2008).

INVITED TALKS

1. APS March Meeting 2017, New Orleans, Louisiana, USA (03/2017), an invited session on "Theory and simulations of defect spin qubits in semiconductors", *Simulations of defect spin qubits in piezoelectric semiconductors.*
2. Electronic Materials and Applications, Orlando, FL, USA (01/2016), *Designing quantum spin defects in ceramic materials for scalable solid-state quantum technologies.*
3. University of Seoul, Seoul, Korea (12/2015), *Study of semiconductor point defects and integration of quantum materials for solid-state quantum technologies.*
4. Busan National University, Busan, Korea (11/2015), *Spin defects in semiconductors for solid-state quantum information processing and nano-scale sensing.*
5. KAIST, Dae-jeon, Korea (11/2015), *Spin defects in semiconductors for solid-state quantum information processing and nano-scale sensing.*

DEPARTMENTAL TALKS

1. University of Chicago, Chicago, IL, USA (11/2015), MRSEC Engineering Quantum Materials & Interaction Series, *Computational modeling of spin defects in semiconductors for scalable solid-state quantum technologies.*
2. University of Chicago, IL, USA (07/2015), Computations in Science seminar, *First-principles computational modeling of defect spins in semiconductors for solid-state quantum information processing.*
3. The University of Texas at Austin, Austin, TX, USA (09/2011), Condensed matter seminar, *Superexchange interaction and strain-induced ferromagnetism in $LaCoO_3$: ab initio study.*